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On computing ``accurate'' derivatives of Equation-of-State variables

A. I. Shestakov

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On computing "accurate" derivatives of Equation-of-State variables*

Aleksei I. Shestakov
Lawrence Livermore National Laboratory
Livermore CA 94550

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Abstract

We analyze a log-log interpolant for 2D EOS lookups, where the EOS independent variables are, say, T and ρ. If the data $f(T_i, \rho_j)$ are in the form of a power law, even locally, the interpolant is exact. It and its derivatives are continuous. Derivatives are computed by analytically differentiating the interpolant. The partial $\partial f/\partial \rho$ is a continuous function of T. Similarly, $\partial f/\partial T$ is continuous wrt ρ. For a sufficiently fine grid in, e.g., T, the discontinuity of $\partial f/\partial T$ is of order ϵ^2, where $T_{i-1}/T_i = 1 - \epsilon$.

1 Warning!

This is an *incomplete* working document.

It has not gone through Review & Release.

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2 Nomenclature

Unless noted otherwise, symbols have the following meaning:

α_T, α_ρ – powers for log-log interpolant
e – specific energy
f – stand-in for energy or pressure
i – energy or temperature index

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I	– total number of i indexes
j	– density index
J	– total number of j indexes
p	– pressure
T	– temperature
τ	– temperature T_{i-1}/T_i ratio
ρ	– mass density
r	– density ρ_{j-1}/ρ_j ratio
Δt	– timestep

3 Introduction

This note grew out of difficulties encountered running a radiation hydrodynamic code with a user-supplied Equation-of-State (EOS). Although the code typically runs using a variety of EOS libraries, it also has an option for the user to supply his/her own. All (?) that's required is to provide energy e and pressure p as functions of temperature T and density ρ *as well as* the four derivatives, e.g., $\partial e/\partial \rho$. The derivatives, presumably, are used to obtain the sound speed in order to compute a stable timestep Δt. (The hydrodynamic package is temporally explicit.)

In our simulations, initially the code ran well, for thousands of steps. The timestep is set by choosing the smallest from a collection supplied by the individual packages (hydrodynamics, radiation.) Apparently, late in time, the hydrodynamic package's Δt is chosen. Unfortunately, that timestep, although by then the smallest, was still too large. The run developed wrinkles reminiscent of violating the Courant condition; first in pressure and velocity, then spreading to density and temperature. The only way to eliminate the "ringing" was by manually reducing Δt.

The EOS in question comes in non-standard form. Text files supply the ratios T/e and $p/\rho e$ on a rectangular grid. The independent variables (equally log-spaced 1D arrays) are density ρ_j and energy e_i (not temperature T_i) where $i = 1, \ldots, I$ and $j = 1, \ldots, J$. We inverted the tables; replaced e_i with temperature T_i and created 2D arrays $p_{i,j}$ and $e_{i,j}$. Luckily, at both the lowest and highest (original) energies e_i, the T/e and $p/\rho e$ ratios are independent of density. Hence, the "edges" of the inverted T_i, ρ_j grid coincide with the original. The ρ_j grid is not changed. The dimension of the new 1D T_i array is the same as the original e_i array, and is also equally log-spaced, i.e., $T_{i-1}/T_i = \tau$, a constant. The inverted $p_{i,j}$ and $e_{i,j}$ values are generated by bilinearly log-interpolating the original T/e and $p/\rho e$ ratios. Derivatives, such as $\partial e/\partial \rho$, were generated on the same inverted (T_i, ρ_j) using second order divided differences; one-sided, first order on the edges.

The derivatives we originally supplied were apparently inaccurate. This note describes an alternative. Derivatives are computed by analytically differentiating the (log-log) interpolant. In a sense, such derivatives are "exact."

4 Code requirements; interpolant

To comply with code requirements, at initialization, 1D arrays T_i and ρ_j (of size I and J, resp.,) and 2D arrays $p_{i,j}$ and $e_{i,j}$ (of size $I \times J$) are read in. Pressures and energies are computed as follows. For each T and ρ, a lookup function supplies indexes i and j into the EOS table s.t.,

$$T_{i-1} \leq T < T_i \text{ and } \rho_{j-1} \leq \rho < \rho_j \,.$$

We then calculate powers

$$\alpha_T = \alpha_T(T) \doteq \frac{\log(T/T_i)}{\log(T_{i-1}/T_i)} \text{ and } \alpha_\rho = \alpha_\rho(\rho) \doteq \frac{\log(\rho/\rho_j)}{\log(\rho_{j-1}/\rho_j)} \,. \tag{1}$$

Thus, $T = T_{i-1}^{\alpha_T} T_i^{1-\alpha_T}$ and $\rho = \rho_{j-1}^{\alpha_\rho} \rho_j^{1-\alpha_\rho}$.

The powers α_T and α_ρ define the interpolant. If $f_{i,j}$ represents either $e_{i,j}$ or $p_{i,j}$, the interpolated value

$$\begin{aligned} \log f \;\; = \;\; & \alpha_T \alpha_\rho \log f_{i-1,j-1} + (1-\alpha_T)\alpha_\rho \log f_{i,j-1} + \\ & (1-\alpha_T)(1-\alpha_\rho) \log f_{i,j} + \alpha_T(1-\alpha_\rho) \log f_{i-1,j} \,. \end{aligned} \tag{2}$$

There are two alternate expressions,

$$\log f = \log(f_{i-1,j}^{\alpha_T} \, f_{i,j}^{1-\alpha_T}) + \alpha_\rho L_T \tag{3}$$

$$\log f = \log(f_{i,j-1}^{\alpha_\rho} \, f_{i,j}^{1-\alpha_\rho}) + \alpha_T L_\rho \,, \tag{4}$$

where L_T and L_ρ, functions of only α_T and α_ρ, resp., may be written as

$$L_T = \log(f_{i,j-1}/f_{i,j}) + \alpha_T L_{i,j} \quad \text{and} \quad L_\rho = \log(f_{i-1,j}/f_{i,j}) + \alpha_\rho L_{i,j} \,, \tag{5}$$

where

$$L_{i,j} = \log\left(\frac{f_{i-1,j-1} \, f_{i,j}}{f_{i-1,j} \, f_{i,j-1}}\right) .$$

Hence, constituents of L_T and L_ρ, e.g., $L_{i,j}$, are "edge-" and "cell-centered" data on the EOS (T_i, ρ_j) grid; hence, can be pre-computed.

The Eq.(2) interpolant has the convenient feature that if the data are in the form of a power law, i.e., if $f = a\rho^b T^c$, for constant a, b, c, even locally, then Eq.(2) returns the exact value.

Derivatives are computed by differentiating the interpolant. Since L_T is independent of α_ρ and L_ρ is independent of α_T,

$$\frac{\partial f}{\partial \rho} = f L_T \frac{\partial \alpha_\rho}{\partial \rho} = \frac{f L_T/\rho}{\log(\rho_{j-1}/\rho_j)} \tag{6}$$

and

$$\frac{\partial f}{\partial T} = f L_\rho \frac{\partial \alpha_T}{\partial T} = \frac{f L_\rho / T}{\log(T_{i-1}/T_i)} \,. \tag{7}$$

Equations (6) and (7) hold inside an EOS (T, ρ) cell with "upper" indexes (i, j).

For fixed ρ, $\partial f/\partial \rho$ is a continuous function of T. The assertion may be proved by brute force or by recalling the definition,

$$\frac{\partial f(T,\rho)}{\partial \rho} = \lim_{\Delta\rho \to 0} \frac{f(T, \rho + \Delta\rho) - f(T,\rho)}{\Delta\rho} \,.$$

Since $f(T, \rho)$ is a continuous function of T, so is $f(T, \rho + \Delta\rho)$. The difference of continuous functions is a continuous function, Q.E.D.

Similarly, for fixed T, $\partial f/\partial T$ is a continuous function of ρ. We consider continuity of the other derivatives in the next section.

5 Equally log-spaced data

In our case, the (T_i, ρ_j) EOS grid is equally log-spaced. Hence, if we define constants $r = \rho_{j-1}/\rho_j$ and $\tau = T_{i-1}/T_i$, the derivatives become

$$\partial f/\partial T = f L_\rho/(T \, \log \tau) \;\text{ and }\; \partial f/\partial \rho = f L_T/(\rho \, \log r) \,. \tag{8}$$

We now consider the continuity of $\partial f/\partial T$ wrt T. Equation (8) holds inside a cell with "upper indexes" i and j. For continuity wrt T, we compare the expression across an i "line," i.e., across (i, j) and $(i + 1, j)$ cells. Equation (8) implies we need only check continuity of L_ρ. For the (i, j) cell, as $T \to T_i$ (from the left), Eq.(5) implies,

$$L_\rho \to \log(f_{i-1,j}/f_{i,j}) + \alpha_\rho L_{i,j} \doteq L_\rho^- \,.$$

And for the $(i + 1, j)$ cell, as $T \to T_i$ (from the right),

$$L_\rho \to \log(f_{i,j}/f_{i+1,j}) + \alpha_\rho L_{i+1,j} \doteq L_\rho^+ \,.$$

Continuity depends on the difference,

$$L_\rho^+ - L_\rho^- = \log F_{i,j} + \alpha_\rho \log(F_{i,j-1}/F_{i,j}) \,,$$

where the grid function

$$F_{i,j} = f_{i,j}^2/(f_{i+1,j}\, f_{i-1,j}) \,.$$

If the data are in the form of a power law, i.e., if $f_{i,j} = a T_i^b \rho_j^c$ for constants a, b and c, $F_{i,j} = 1$ for all i and j; hence, $L_\rho^+ - L_\rho^- = 0$, which proves continuity wrt T. A similar argument applies to the continuuity of $\partial f/\partial \rho$ wrt ρ.

For data *not* in the form of a power law, using Taylor's theorem,

$$\begin{aligned} f_{i-1,j} &= f_{i,j} + \Delta T_-(\partial f/\partial T)_{i,j} + \mathcal{O}(\Delta T_-^2) \\ f_{i+1,j} &= f_{i,j} + \Delta T_+(\partial f/\partial T)_{i,j} + \mathcal{O}(\Delta T_+^2)\,. \end{aligned}$$

For the equally log-spaced T mesh,

$$\Delta T_- = T_i(\tau - 1) \quad \text{and} \quad \Delta T_+ = T_i(\tau^{-1} - 1)\,.$$

Hence,

$$F_{i,j} = 1/[1 + T_i\,(\partial f/\partial T)_{i,j}\, f_{i,j}^{-1}\,(\tau-1)^2/\tau + \mathcal{O}(\Delta T^2)]\,.$$

Assuming a sufficiently fine grid, s.t., $\tau = 1 - \epsilon$, with ϵ small,

$$F_{i,j} = 1 - T_i\,(\partial f/\partial T)_{i,j}\, f_{i,j}^{-1}\,\epsilon^2 + \mathcal{O}(\epsilon^2)\,.$$

In other words, $F_{i,j} = 1 + \mathcal{O}(\epsilon^2)$. Consequently, $F_{i,j}/F_{i,j-1}$ also equals $1+$ $+\mathcal{O}(\epsilon^2)$. Thus,

$$L_\rho^+ - L_\rho^- = \mathcal{O}(\epsilon^2) + \alpha_\rho\,\mathcal{O}(\epsilon^2) = \mathcal{O}(\epsilon^2)\,,$$

since $0 \le \alpha_\rho < 1$.

Hence, for a sufficiently fine grid of the independent variable T_i, the discontinuity of $\partial f/\partial T$ wrt T, is of order ϵ^2, where $T_{i-1}/T_i = 1 - \epsilon$.

A similar argument holds for the discontinuity of $\partial f/\partial \rho$ wrt ρ. Unfortunately, for our EOS, while the T_i grid is relatively fine ($\epsilon_T = 0.14$), the ρ_j grid is relatively coarse ($\epsilon_\rho = 0.9$). However, the discontinuity is partly offset by the relatively slow variation e and p have wrt ρ.[1]

6 Conclusion

We analyzed a log-log interpolant for 2D EOS lookups, where the EOS independent are T and ρ. If the data $f(T_i, \rho_j)$ are in the form of a power law, even locally, the interpolant is exact and it and its derivatives are continuous. The interpolant of $\partial f/\partial \rho$ is a continuous function of T. Similarly, $\partial f/\partial T$ is a continuous function ρ. For a sufficiently fine grid in, say, T, the discontinuity of $\partial f/\partial T$ is of order ϵ^2, where $T_{i-1}/T_i = 1 - \epsilon$.

7 Acknowledgment

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[1] Generally, the EOS is closely approximated by an ideal gas law, where e is independent of ρ and $p \propto \rho$. Thus, it may be better to tabulate $q = p/\rho$ instead of p. Then, since q varies slowly with ρ, $\partial q/\partial \rho$ should be small. And the required derivative $\partial p/\partial \rho = q + \rho \partial q/\partial \rho$.